

1,1,2,2-Tetrahydroperfluoro-1-decanol
678-39-7 | DTXSID7029904

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 154 °C

Global applicability domain: Outside

Local applicability domain index: 2.63e-01

Confidence level: 6.87e-01

Nearest Neighbors from the Training Set

Image not found

1-Octanol,
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-
pentadecafluoro-

Measured: 161

Predicted: 156

Image not found

Methyl perfluorooctanoate

Measured: 158

Predicted: 151

Image not found

1-Decene,
3,3,4,4,5,5,6,6,7,7,8,8,9,10,10,10-
heptadecafluoro-

Measured: 150

Predicted: 148

Image not found

Perflunafene

Measured: 142

Predicted: 141